# **Product data sheet**



MedKoo Cat#: 535178		
Name: NP19		
CAS: 2377916-66-8		ľ
Chemical Formula: C <sub>33</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>4</sub>		
Exact Mass: 554.1972		
Molecular Weight: 555.	(	
Product supplied as:	Powder	
Purity (by HPLC):	$\geq 98\%$	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.	
	In solvent: -80°C 3 months; -20°C 2 weeks.	

## 1. Product description:

NP19 is an inhibitor of the protein-protein interaction between programmed cell death 1 (PD-1) and its ligand PD-L1 (IC50 = 12.5 nM in a homogenous time-resolved fluorescence (HTRF) assay). It increases IFN- $\gamma$  production by isolated human peripheral blood mononuclear cells (PBMCs) in co-culture with anti-CD3 single-chain variable fragment- and PD-L1-expressing Hep3B hepatoma cells (EC50 = ~3  $\mu$ M). NP19 (25, 50, and 100 mg/kg) reduces tumor growth in a B16/F10 murine melanoma model and an H22 murine hepatocellular carcinoma model.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	30.0	54.05
DMSO	16.0	28.83

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.80 mL	9.01 mL	18.02 mL
5 mM	0.36 mL	1.80 mL	3.60 mL
10 mM	0.18 mL	0.90 mL	1.80 mL
50 mM	0.04 mL	0.18 mL	0.36 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

## 6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

Cheng B, Ren Y, Niu X, Wang W, Wang S, Tu Y, Liu S, Wang J, Yang D, Liao G, Chen J. Discovery of Novel Resorcinol Dibenzyl Ethers Targeting the Programmed Cell Death-1/Programmed Cell Death-Ligand 1 Interaction as Potential Anticancer Agents. J Med Chem. 2020 Aug 13;63(15):8338-8358. doi: 10.1021/acs.jmedchem.0c00574. Epub 2020 Jul 30. PMID: 32667799.

#### In vivo study

Cheng B, Ren Y, Niu X, Wang W, Wang S, Tu Y, Liu S, Wang J, Yang D, Liao G, Chen J. Discovery of Novel Resorcinol Dibenzyl Ethers Targeting the Programmed Cell Death-1/Programmed Cell Death-Ligand 1 Interaction as Potential Anticancer Agents. J Med Chem. 2020 Aug 13;63(15):8338-8358. doi: 10.1021/acs.jmedchem.0c00574. Epub 2020 Jul 30. PMID: 32667799.

## 7. Bioactivity

Biological target:

PD-1/PD-L1-IN-NP19 is a PD-1/PD-L1 inhibitor, with an IC<sub>50</sub> of 12.5 nM for human PD-1/PD-L1 interaction.

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In vitro activity

Compound NP19 inhibited the human PD-1/PD-L1 interaction with IC<sub>50</sub> values of 12.5 nM in homogeneous time-resolved fluorescence (HTRF) binding assays. In addition, NP19 dose-dependently elevated IFN- $\gamma$  production in a coculture model of Hep3B/OS-8/hPD-L1 and CD3 T cells.

Reference: J Med Chem. 2020 Aug 13;63(15):8338-8358. https://pubmed.ncbi.nlm.nih.gov/32667799/

## In vivo activity

Furthermore, NP19 displayed significant in vivo antitumor efficacy in two different mouse models of cancer (a melanoma B16-F10 tumor model and an H22 hepatoma tumor model). Moreover, H&E staining and flow cytometry data suggested that NP19 activated the immune microenvironment in the tumor, which may contribute to its antitumor effects.

Reference: J Med Chem. 2020 Aug 13;63(15):8338-8358. https://pubmed.ncbi.nlm.nih.gov/32667799/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.